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Structure and Energy Stability of Metal Nanoparticles¹ HECTOR BARRON, University of Texas at San Antonio, JUAN PEDRO PALOMARES-BAEZ, Instituto Potosino de Investigacion Cientifica y Tecnologica, JESUS VELAZQUEZ-SALAZAR, University of Texas at San Antonio, JOSE LUIS RODRIGUEZ-LOPEZ, Instituto Potosino de Investigacion Cientifica y Tecnologica, MIGUEL JOSE-YACAMAN, University of Texas at San Antonio, UNIVERSITY OF TEXAS AT SAN ANTONIO COLLABORATION, INSTITUTO POTOSINO DE INVESTIGACION CIENTUFICA Y TECNOLOGICA COLLABORATION — In this work we present a theoretical model for the structural evolution and energy stability for metal nanoparticles from the small (1-2 nm) to the big (~ 50 nm) size ranges. We have found that the appearances of structural lattice defects as well as surface reconstructions are important factors that highly influence the growth process. A simple assembly model for a path transformation for metal nanoparticles is presented and compare with experimental evidence.

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